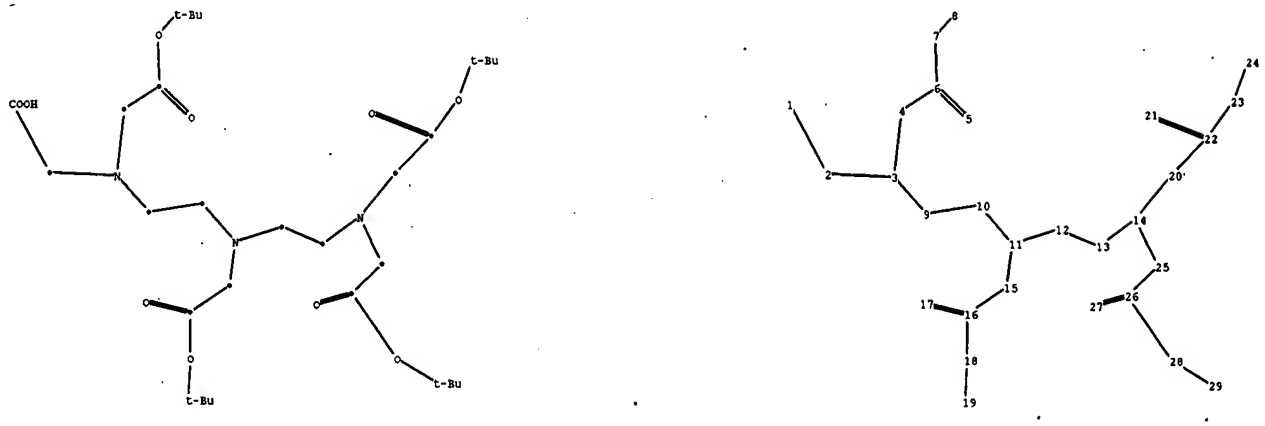
EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	3219	"424/184.1".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:17
L2	868	"530/403".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:17
L3	853	"560/41".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:18
L4	133	((WILLIAM) near2 (MCBRIDE)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:18
L5	150	((DAVID) near2 (GOLDENBERG)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:18
L6	42	((WILLIAM) near2 (MCBRIDE)).INV.	EPO; JPO; DERWENT	OR	ON	2007/10/29 16:18
L7	84	((DAVID) near2 (GOLDENBERG)).INV.	EPO; JPO; DERWENT	OR	ON	2007/10/29 16:19
L10	583	L2 AND @AY<"1998"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:21
L11	1030	L1 AND @AY<"1998"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:21
L12	404	L3 AND @AY<"1998"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:26
L13	4	(("6962702") or ("7074405") or ("7138103") or ("7052872")).PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2007/10/29 16:59
L14	4	(("5695737") or ("6080785") or ("6607710") or ("7052872") or ("2006264669")).PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2007/10/29 17:02
L15	5	(("5695737") or ("6080785") or ("6607710") or ("7052872") or ("20060264669")).PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2007/10/29 17:02
L16	2	("6080785").URPN.	USPAT	OR	ON	2007/10/29 17:03

C:\Program Files\Stnexp\Queries\2007 cases\10766470\molecule V cl118.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29

chain bonds :
1-2 2-3 3-4 3-9 4-6 5-6 6-7 7-8 9-10 10-11 11-12 11-15 12-13 13-14 14-20 14-25 15-16 16-17 16-18 18-19 20-22 21-22 22-23 23-24 25-26 26-27 26-28 28-29

exact/norm bonds :
2-3 3-4 3-9 5-6 6-7 10-11 11-12 11-15 13-14 14-20 14-25 16-17 16-18 21-22 22-23 26-27 26-28

exact bonds :
1-2 4-6 7-8 9-10 12-13 15-16 18-19 20-22 23-24 25-26 28-29

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS

10/776470 Therapeutic n DiagnosticConjugates

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAMLL1621

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 02	LMEDLINE coverage updated
NEWS 3	JUL 02	SCISEARCH enhanced with complete author names
NEWS 4	JUL 02	CHEMCATS accession numbers revised
NEWS 5	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 6	JUL 16	CAplus enhanced with French and German abstracts
NEWS 7	JUL 18	CA/CAplus patent coverage enhanced
NEWS 8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9	JUL 30	USGENE now available on STN
NEWS 10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 11	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 12	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 13	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 14	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 15	AUG 27	USPATOLD now available on STN
NEWS 16	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 17	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 18	SEP 13	FORIS renamed to SOFIS
NEWS 19	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 20	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 21	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 22	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 23	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 24	OCT 19	BEILSTEIN updated with new compounds

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 OCT 2007 HIGHEST RN 951754-22-6
DICTIONARY FILE UPDATES: 28 OCT 2007 HIGHEST RN 951754-22-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\2007 cases\10766470\molecule V cl118.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 16:56:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

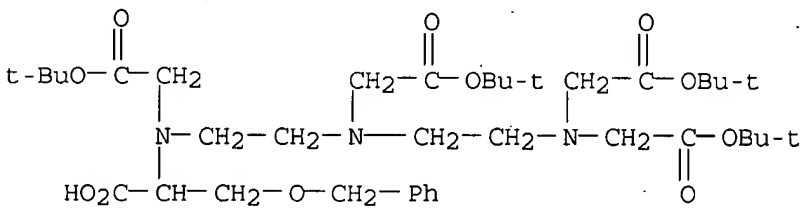
100.0% PROCESSED 14 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 56 TO 504
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d sca

L2 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 4-carboxy-5,8,11-tris[2-(1,1-dimethylethoxy)-2-oxoethyl]-1-phenyl-, 13-(1,1-dimethylethyl) ester (9CI)
MF C38 H63 N3 O11



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l1 sss full
FULL SEARCH INITIATED 16:56:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 287 TO ITERATE

100.0% PROCESSED 287 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

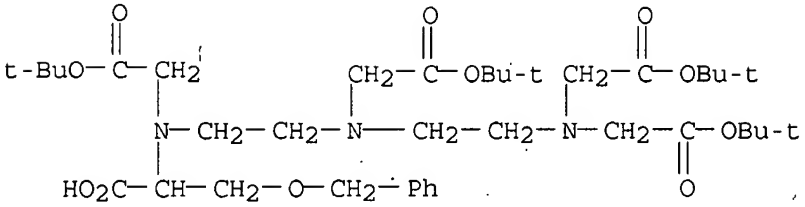
L3 5 SEA SSS FUL L1

=> d sca str rn
INVALID SCAN FIELD FOR FILE 'REGISTRY'

One or more of the display fields specified are not valid with DISPLAY SCAN in the current file. Enter HELP DSCAN at the arrow prompt (=>) for the list of fields that may be used when scanning the answers.

=> d sca

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 4-carboxy-5,8,11-tris[2-(1,1-dimethylethoxy)-2-oxoethyl]-1-phenyl-, 13-(1,1-dimethylethyl) ester (9CI)
MF C38 H63 N3 O11

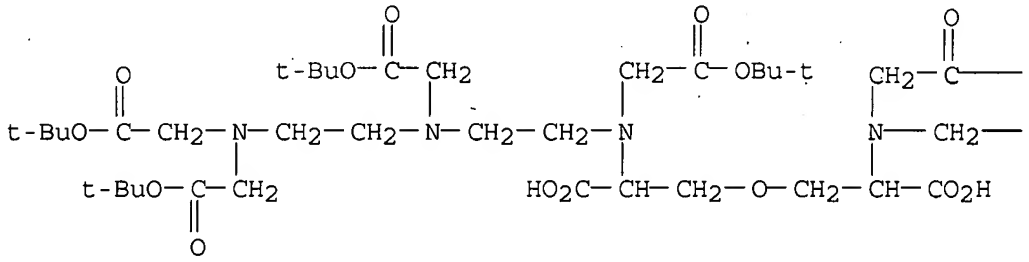


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

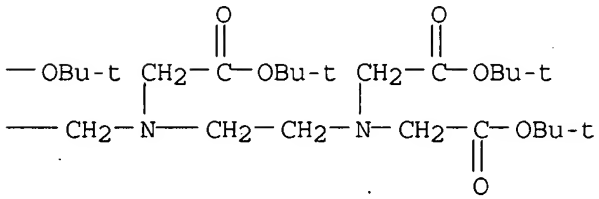
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 11-Oxa-2,5,8,14,17,20-hexaazaheneicosane-1,9,13,21-tetracarboxylic acid, 2,5,8,14,17,20-hexakis[2-(1,1-dimethylethoxy)-2-oxoethyl]-, 1,21-bis(1,1-dimethylethyl) ester (9CI)
MF C62 H112 N6 O21

PAGE 1-A

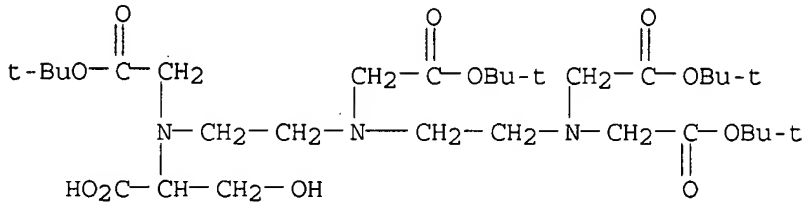


PAGE 1-B



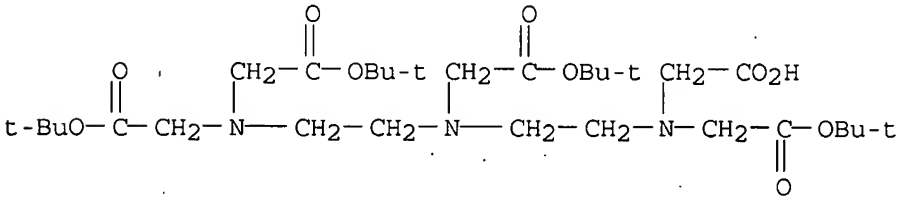
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 3-Oxa-6,9,12-triazatetradecan-14-oic acid, 6-(1-carboxy-2-hydroxyethyl)-9,12-bis[2-(1,1-dimethylethoxy)-2-oxoethyl]-2,2-dimethyl-4-oxo-, 14-(1,1-dimethylethyl) ester (9CI)
MF C31 H57 N3 O11



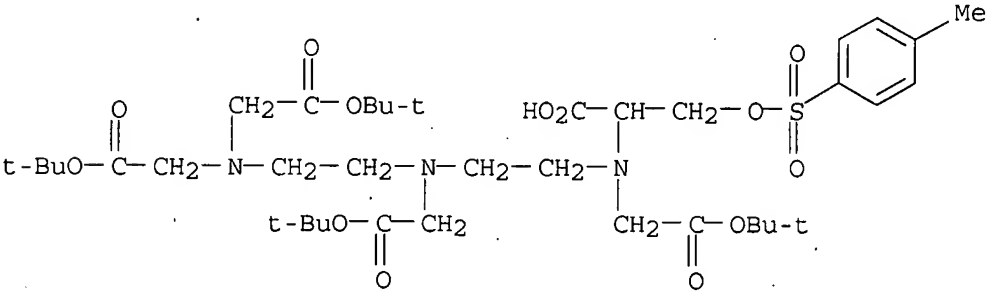
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 3-Oxa-6,9,12-triazatetradecan-14-oic acid, 12-(carboxymethyl)-6,9-bis[2-(1,1-dimethylethoxy)-2-oxoethyl]-2,2-dimethyl-4-oxo-, 14-(1,1-dimethylethyl) ester
MF C30 H55 N3 O10



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 3-Oxa-6,9,12-triazatetradecan-14-oic acid, 6-[1-carboxy-2-[[(4-methylphenyl)sulfonyl]oxy]ethyl]-9,12-bis[2-(1,1-dimethylethoxy)-2-oxoethyl]-2,2-dimethyl-4-oxo-, 14-(1,1-dimethylethyl) ester (9CI)
MF C38 H63 N3 O13 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file hcapl

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.45	173.66

FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 29 Oct 2007 VOL 147 ISS 19
FILE LAST UPDATED: 28 Oct 2007 (20071028/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007)

FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 5 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007

=> s l3
L4 20 L3

=> d l3 1-20 ibib abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d l4 1-20 ibib abs

L4 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1224889 HCAPLUS
DOCUMENT NUMBER: 145:505757
TITLE: Method for manufacturing diethylenetriaminepentaacetic acid derivatives

INVENTOR(S): Lee, Te-Wei; Yang, Chia-Hsi; Ho, Yen-Sheng; Lu, Li-Hui; Chen, Shu-Ling
PATENT ASSIGNEE(S): Atomic Energy Council - Institute of Nuclear Energy Research, Taiwan
SOURCE: U.S. Pat. Appl. Publ., 10pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006264669	A1	20061123	US 2005-134397	20050523
JP 2006342105	A	20061221	JP 2005-169511	20050609

PRIORITY APPLN. INFO.: US 2005-134397 A 20050523
OTHER SOURCE(S): MARPAT 145:505757

AB The invention relates to regioselective hydrolysis of diethylenetriaminepentaacetic acid (DTPA) tetraalkyl esters by using a metal ion as catalyst to obtain monoreactive DTPA tetraalkyl esters. Thus, DTPA pentaethyl ester (prepared from DTPA dianhydride) in aqueous NaOH solution containing CuCl2 was bubbled with H2S and the solution filtered to remove Cu2S to yield 61 % DTPA tetra-Et ester in which the free carboxy group is at the terminal position.

L4 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:495678 HCAPLUS
DOCUMENT NUMBER: 145:140459
TITLE: Phosphorylation State-Responsive Lanthanide Peptide Conjugates: A Luminescence Switch Based on Reversible Complex Reorganization
AUTHOR(S): Tremblay, Matthew S.; Zhu, Qing; Marti, Angel A.; Dyer, Joanne; Halim, Marlin; Jockusch, Steffen; Turro, Nicholas J.; Sames, Dalibor
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Organic Letters (2006), 8(13), 2723-2726
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:140459

AB A luminogenic probe for peptide dephosphorylation has been developed. It consists of a serine-/tyrosine-containing peptide modified on the N-terminus with a tryptophan residue and a DTPA chelate capable of binding Tb3+. The authors propose a mechanistic model for the luminescence enhancement based on the interconversion of monomeric and dimeric lanthanide species, which is affected by the phosphorylation state of the serine or tyrosine residue. The optical switch reports effectively on phosphatase-catalyzed dephosphorylation in vitro.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:487757 HCAPLUS
DOCUMENT NUMBER: 146:402266
TITLE: Development of a 111In-labeled peptide derivative

targeting a chemokine receptor, CXCR4, for imaging tumors
AUTHOR(S): Hanaoka, Hirofumi; Mukai, Takahiro; Tamamura, Hirokazu; Mori, Tomohiko; Ishino, Seigo; Ogawa, Kazuma; Iida, Yasuhiko; Doi, Ryuichiro; Fujii, Nobutaka; Saji, Hideo
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Kyoto University, Yoshida Shimoadachi-cho, Sakyo-ku, Kyoto, 606-8501, Japan
SOURCE: Nuclear Medicine and Biology (2006), 33(4), 489-494
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The chemokine receptor CXCR4 is highly expressed in tumor cells and plays an important role in tumor metastasis. The aim of this study was to develop a radiopharmaceutical for the imaging of CXCR4-expressing tumors in vivo. Based on structure-activity relationships, the authors designed a 14-residue peptidic CXCR4 inhibitor, Ac-TZ14011, as a precursor for radiolabeled peptides. For 111In-labeling, diethylenetriaminepentaacetic acid (DTPA) was attached to the side chain of D-Lys8 which is distant from the residues indispensable for the antagonistic activity. In-DTPA-Ac-TZ14011 inhibited the binding of a natural ligand, stromal cell-derived factor-1α, to CXCR4 in a concentration-dependent manner with IC50 = 7.9 nM (Ac-TZ14011: 1.2 nM). In biodistribution expts., more 111In-DTPA-Ac-TZ14011 accumulated in the CXCR4-expressing tumor than in blood or muscle. Furthermore, the tumor-to-blood and tumor-to-muscle ratios were significantly reduced by coinjection of Ac-TZ14011, indicating a CXCR4-mediated accumulation in tumor. These findings suggested that 111In-DTPA-Ac-TZ14011 would be a potential agent for the imaging of CXCR4 expression in metastatic tumors in vivo.
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:951424 HCAPLUS
DOCUMENT NUMBER: 143:422550
TITLE: Synthesis of DTPA-conjugated (1,4)-linked 2-amino-glycosides varying in the anomeric configuration and their MRI contrast effect
AUTHOR(S): Tanaka, Hiroshi; Ando, Yoshio; Wada, Masatoshi; Takahashi, Takashi
CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Science and Engineering, Tokyo Institute of Technology, Tokyo, Meguro, 152-8552, Japan
SOURCE: Organic & Biomolecular Chemistry (2005), 3(18), 3311-3328
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The efficient synthesis of diethylenetriamine-N,N,N',N'',N''-penta-acetic acid (DTPA)-conjugated oligosaccharides composed of α- and/or β-linked tri to mono-glucosamines is described. Gd(III) complex with DTPA-conjugated chitotriitol has been reported to be an effective MRI contrast agent. In order to elucidate the structure-property relationships, we planned to synthesize the DTPA-conjugated 2-amino-tri-, di-, and monosaccharides varying in configuration at the anomeric

positions and the C2 position on the reducing end. Our strategy for the synthesis of the DTPA-conjugated oligosaccharides involves O-per-benzyl protected 2-amino-tri-, di-, and monosaccharides as key intermediates. The 2-amino-glycosides were prepared by non-selective glycosidation of 2-azido-2-deoxy-glycosyl donors, followed by separation of two anomeric isomers. Although the synthesis involves separation of the stereoisomers, it circumvents not only the careful tuning of reaction conditions, but also the time-consuming preparation of glycosyl donors attached to different protecting groups. The protected 2-amino-glycosides were converted to the fully deprotected DTPA-conjugated tri- to monosaccharides by the same operation. MRI phantom study using the Gd(III) complexes of DTPA-conjugated oligosaccharides indicates that the number of the monosaccharide units was critical for enhancing the relative signal intensity of water protons per Gd, and various stereoisomers would be candidate scaffolds for MRI contrast agents.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:235070 HCAPLUS
DOCUMENT NUMBER: 142:293787
TITLE: Somatostatin analogs and metal complexes for MRI diagnosis and treatment of tumors
INVENTOR(S): Saito, Hiroshi; Saji, Hideo; Arano, Yasushi; Iwafuji, Akimasa; Mifune, Masaki; Mukai, Takahiro; Akisawa, Hiroyuki; Takimoto, Yamato
PATENT ASSIGNEE(S): Nihon Mediphysics Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005068046	A	20050317	JP 2003-297606	20030821
PRIORITY APPLN. INFO.:			JP 2003-297606	20030821

OTHER SOURCE(S): MARPAT 142:293787
AB Somatostatin analogs (I, RNHCH(CH2X)CO-Cys-A-dTrp-Lys-B-Cys-Y wherein R = chelator residue. including DTPA, DOTA, etc.; X = carboxyl, aminophenyl, naphthyl; Y = Thr-OH, Thr-NH2, Trp-NH2; A = Phe, Tyr; B = Thr, Val) and metal complexes are claimed for MRI diagnosis and treatment of tumors by targeting somatostatin receptors. I-111In complexes were prepared, and their pharmacokinetics in tissues were determined

L4 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:15791 HCAPLUS
DOCUMENT NUMBER: 142:120462
TITLE: Therapeutic and diagnostic conjugates for use with multispecific antibodies
INVENTOR(S): Mcbride, William J.; Goldenberg, David M.; Noren, Carl; Hansen, Hans J.
PATENT ASSIGNEE(S): Immunomedics, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 53 pp., Cont.-in-part of U.S. Ser. No. 150,654.
CODEN: USXXCO
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005002945	A1	20050106	US 2004-776470	20040211
US 7074405	B1	20060711	US 1999-337756	19990622
US 7052872	B1	20060530	US 1999-382186	19990823
US 2002006379	A1	20020117	US 2001-823746	20010403
US 6962702	B2	20051108		
US 2003198595	A1	20031023	US 2002-150654	20020517
US 7138103	B2	20061121		
AU 2005211754	A1	20050825	AU 2005-211754	20050211
CA 2555666	A1	20050825	CA 2005-2555666	20050211
WO 2005077071	A2	20050825	WO 2005-US4177	20050211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1720575	A2	20061115	EP 2005-726492	20050211
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
JP 2007528372	T	20071011	JP 2006-553216	20050211

PRIORITY APPLN. INFO.:

US 1998-90142P	P	19980622
US 1998-104156P	P	19981014
US 1999-337756	A2	19990622
US 1999-382186	B2	19990823
US 2001-823746	A2	20010403
US 2002-150654	A2	20020517
US 2004-776470	A	20040211
WO 2005-US4177	W	20050211

OTHER SOURCE(S): MARPAT 142:120462

AB Disclosed are compds. that include two or more haptens conjugated by a spacer or a carrier. The haptens may include diethylenetriaminepentaacetate (DTPA), histamine-succinyl-glutamine (HSG), or combinations of DTPA and HSG. The compds. also includes an effector mol. which may be conjugated to one or more of the haptens, the spacer/carrier, or both. The effector mol. may be conjugated by a number of linkages including an ester linkage, an imino linkage, an amino linkage, a sulfide linkage, a thiosemicarbazone linkage, a semicarbazone linkage, an oxime linkage, an ether linkage, or combinations of these linkages. Also disclosed are methods of synthesizing the compds. and/or precursors of the compds.

L4 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:795339 HCAPLUS
DOCUMENT NUMBER: 141:421892
TITLE: De Novo Designed Peptidic Redox Potential Probe: Linking Sensitized Emission to Disulfide Bond

Formation
AUTHOR(S): Lee, Kyung; Dzubeck, Valerie; Latshaw, Lauren; Schneider, Joel P.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716-2522, USA
SOURCE: Journal of the American Chemical Society (2004), 126(42), 13616-13617
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:421892
AB The design and utility of a peptidic probe capable of accurately measuring environmental redox potential via sensitized emission has been prepared This probe is characterized by long-lived luminescence (millisecond), nanomolar detection limits, and a probe reduction potential of -0.243 V.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:144091 HCAPLUS
DOCUMENT NUMBER: 141:391077
TITLE: Effect of carboxylation of N-terminal phenylalanine of 111In-DTPA (diethylenetriaminepentaacetic acid)-octreotide on accumulation of radioactivity in kidney
AUTHOR(S): Akizawa, Hiromichi; Takimoto, Hirokazu; Saito, Madoka; Iwado, Akimasa; Mifune, Masaki; Saito, Yutaka; Uehara, Tomoya; Arano, Yasushi; Mukai, Takahiro; Hanaoka, Hirofumi; Saji, Hideo
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Okayama University, Okayama, 700-8530, Japan
SOURCE: Biological & Pharmaceutical Bulletin (2004), 27(2), 271-272
CODEN: BPBLEO; ISSN: 0918-6158
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB For purpose of reducing renal accumulation of radioactivity of a known radiopharmaceutical agent, i.e., 111In-DTPA (diethylenetriaminepentaacetic acid)-D-Phe1-octreotide, a derivative in which p-carboxy-L-phenylalanine is substituted for D-Phe1 was synthesized. Biodistribution study of the resultant compound having carboxy-substituted L-Phe1 revealed that the renal accumulation was significantly lower than that of control compound having unsubstituted L-Phe1, demonstrating that the presence of neg. charge on the N-terminal amino acid of octreotide is effective to reduce the renal accumulation. This effect can be attributed to the reduction of lipophilicity and also the repulsive force arisen from the neg. charge of renal brush border membrane.
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:959352 HCAPLUS
DOCUMENT NUMBER: 138:142331
TITLE: Design, Synthesis, and Evaluation of Gadolinium Cationic Lipids As Tools for Biodistribution Studies of Gene Delivery Complexes

AUTHOR(S): Leclercq, Francoise; Cohen-Ohana, Mirit; Mignet, Nathalie; Sbarbati, Andrea; Herscovici, Jean; Scherman, Daniel; Byk, Gerardo
CORPORATE SOURCE: Department of Chemistry, Laboratory of Peptidomimetics and Genetic Chemistry, Bar Ilan University, Ramat Gan, 52900, Israel
SOURCE: Bioconjugate Chemistry (2003), 14(1), 112-119
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Gadolinium-chelating cationic lipids have been synthesized to obtain lipoplexes with MRI contrast properties. These compds. were designed to follow the biodistribution of synthetic DNA for gene delivery by NMR imaging. The lipid MCO-I-68 was synthesized, and chelate complexes with gadolinium were formed and characterized in terms of physicochem. and DNA binding properties. The transfection activity of MCO-I-68-Gd/DNA complexes was assayed in vitro on NIH 3T3. Different formulations of the product were tested. When up to 5% of the gadolinium lipid complexes were co-formulated with the cationic lipid RPR120535 used as a reference, the transfection levels were maintained as compared to RPR120535 alone. To date, only a liposomal formulation of a gadolinium-cationic lipid chelate without DNA had been observed using magnetic resonance imaging. In vivo intratumoral administration of MCO-I-68-Gd/DNA lipoplexes to tumor model led to an important increase of the NMR signal. It was demonstrated that the new complexes also acted as transfection carriers when they were formulated from liposomes.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:407215 HCAPLUS
DOCUMENT NUMBER: 136:81993
TITLE: Significance of 111In-DTPA chelate in renal radioactivity levels of 111In-DTPA-conjugated peptides
AUTHOR(S): Akizawa, H.; Arano, Y.; Mifune, M.; Iwado, A.; Saito, Y.; Uehara, T.; Ono, M.; Fujioka, Y.; Ogawa, K.; Kiso, Y.; Saji, H.
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Okayama University, Tsushima-naka, Okayama, 700-8530, Japan
SOURCE: Nuclear Medicine and Biology (2001), 28(4), 459-468
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Metabolic studies of 111In-DTPA-labeled polypeptides and peptides showed that the radiolabeled (poly)peptides generated 111In-DTPA-adducts of amino acid that possess long residence times in the lysosomal compartment of the tissues where (poly)peptides accumulated. However, a recent study suggested that metal-chelate-methionine (Met) might possess in vivo behaviors different from metal-chelate adducts of other amino acids. In this study, to elucidate whether some biol. characteristics of Met may accelerate the renal elimination rate of 111In-DTPA-adduct of Met into urine, 111In-DTPA-Met1-octreotide was synthesized and the renal handling of 111In-DTPA-Met was investigated using 111In-DTPA-1-Phe1-octreotide (Phe represents phenylalanine), which was reported previously, as a reference Both 111In-DTPA-conjugated octreotide analogs were stable against 3-h incubation in murine serum at 37°C. Both 111In-DTPA-octreotide

analogs also showed rapid clearance of the radioactivity from the blood and similar accumulation of the radioactivity in the kidney. No significant differences were observed in the renal radioactivity levels from 10 min to 24 h postinjection between the two. Metabolic studies indicated that 111In-DTPA-Met1-octreotide and 111In-DTPA-1-Phe1-octreotide generated 111In-DTPA-adducts of Met and Phe, resp., as the final radiometabolites at similar rates. These findings suggested that the long residence times of the radioactivity in tissues after administration of 111In-DTPA-labeled peptides and polypeptides would be attributed to inherent characteristics of 111In-DTPA chelate.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:279459 HCAPLUS
DOCUMENT NUMBER: 134:292147
TITLE: Bisphosphonic acid derivative and compound thereof labelled with radioactive nuclide
INVENTOR(S): Ito, Osamu; Kanazashi, Nobuhiko; Morishita, Aki; Hara, Masamichi; Kanagawa, Masaru; Watanabe, Yasuko; Itaya, Yoshitoshi
PATENT ASSIGNEE(S): Nihon Medi-Physics Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1092723	A2	20010418	EP 2000-308983	20001012
EP 1092723	A3	20010926		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001114792	A	20010424	JP 1999-288952	19991012
CA 2322936	A1	20010412	CA 2000-2322936	20001011
US 6607710	B1	20030819	US 2000-686372	20001012
PRIORITY APPLN. INFO.:			JP 1999-288952 A	19991012

OTHER SOURCE(S): MARPAT 134:292147

AB An object of the present invention is to provide a bisphosphonic acid derivative and said bisphosphonic acid derivative being labeled with a radioactive nuclide, which has properties of rapid accumulation to the bone and rapid urinary excretion. The present invention relates to a bisphosphonic acid derivative and said bisphosphonic acid derivative being labeled with a radioactive nuclide, which is represented by the general formula R-Y-A, wherein A is a bisphosphonic acid or a salt thereof, having P-C-P bond; Y is a bonding portion such as a methylene, an amido etc.; R is a group of any one of a polyaminopolycarboxylic acid, an aliphatic carboxylic acid, a mercaptoacetylpolyamino acid or its derivs. and a disubstituted benzene compound where one substituent is a halogen atom or an isotope thereof or an alkyl tin; and the second substituent is a group of any one of compds. of an aminocarboxylic acid, an alkyloarboxylic acid or a substituted-alkylcarboxylic acid, an alkysulfonic acid or a substituted-alkysulfonic acid. The radiolabeled bisphosphonate derivative which has an affinity for bone can be used in diagnosis or therapy of bone diseases.

L4 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:581385 HCAPLUS
DOCUMENT NUMBER: 132:3542
TITLE: Direct solid-phase synthesis of octreotide conjugates: precursors for use as tumor-targeted radiopharmaceuticals
AUTHOR(S): Hsieh, H.-P.; Wu, Y.-T.; Chen, S.-T.; Wang, K.-T.
CORPORATE SOURCE: Institute of Biological Chemistry, Academia Sinica, Nankang, Taiwan
SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(9), 1797-1803
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Somatostatin analogs, such as octreotide, are useful for the visualization and treatment of tumors. Unfortunately, these compds. were produced synthetically using complex and inefficient procedures. Here, the authors describe a novel approach for the synthesis of octreotide and its analogs using p-carboxybenzaldehyde to anchor Fmoc-threoninol to solid phase resins. The reaction of the two hydroxyl groups of Fmoc-threoninol with p-carboxybenzaldehyde was catalyzed with p-toluenesulfonic acid in chloroform using a Dean-Stark apparatus to form Fmoc-threoninol p-carboxybenzacetal in 91% yield. The Fmoc-threoninol p-carboxybenzacetal acted as an Fmoc-amino acid derivative and the carboxyl group of Fmoc-threoninol p-carboxybenzacetal was coupled to an amine-resin via a DCC coupling reaction. The synthesis of protected octreotide and its conjugates were carried out in their entirety using a conventional Fmoc protocol and an autosynthesizer. The acetal was stable during the stepwise elongation of each Fmoc-amino acid as shown by the averaged coupling yield (>95%). Octreotide (74 to 78% yield) and five conjugated derivs. were synthesized with high yields using this procedure, including three radiotherapy octreotides (62 to 75% yield) and two cellular markers (72 to 76% yield). This novel approach provides a strategy for the rapid and efficient large-scale synthesis of octreotide and its analogs for radiopharmaceutical and tagged conjugates.

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:409606 HCAPLUS
DOCUMENT NUMBER: 131:56136
TITLE: Dendritic polymer-saccharide conjugates and their preparation for use in NMR contrast media
INVENTOR(S): Berndorff, Dietmar; Mareski, Peter; Misselwitz, Bernd; Platzek, Johannes; Raduechel, Bernd; Weinmann, Hanns-Joachim
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 54 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

DE 19758105	A1	19990624	DE 1997-19758105	19971218
WO 9932154	A1	19990701	WO 1998-EP7927	19981209
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9922680	A	19990712	AU 1999-22680	19981209
EP 1037672	A1	20000927	EP 1998-966256	19981209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2001526247	T	20011218	JP 2000-525144	19981209
PRIORITY APPLN. INFO.:			DE 1997-19758105 A	19971218
			WO 1998-EP7927 W	19981209

AB The title conjugates, PKm(LZ)n (P = dendritic polymer with 12-150 amino groups; K = metal chelate group as detectable label; L = linker; Z = mono- or oligosaccharide group; m, n = 1-149), are excellent contrast agents for NMR diagnostics, especially for lymphog. These conjugates are accumulated by the lymphatic system adequately for imaging, in some cases even sufficiently for morphol. differentiation of lymph nodes. They are relatively nontoxic, are excreted slowly (>98% in 14 days), and show a high relaxivity which allows their use in low dosages. Thus, a dendritic polyamine with 64 amino groups, of which 38 bore Gd-DTPA chelate groups and 26 were substituted with 1-(4-thioureidophenyl)-α-D-mannopyranosyl groups, when injected i.v. at 200 μmol Gd/kg into rats, was accumulated in the liver, spleen, and especially in the mesenteric and peripheral lymph nodes. Owing to the high relaxivity of this compound in water (17.0 L/mmol s), a dose of ≥10 μmol Gd/kg for i.v. NMR lymphog. is recommended. Preparation of this and other contrast agents from the unsubstituted dendritic polyamines is described.

L4 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1999:53428 HCAPLUS
DOCUMENT NUMBER:	130:125343
TITLE:	Saccharide conjugates, their preparation and use as contrast agents and therapeutic agents
INVENTOR(S):	Mareski, Peter; Platzek, Johannes; Raduechel, Bernd; Berndorff, Dietmar; Weinmann, Hanns-Joachim
PATENT ASSIGNEE(S):	Schering Aktiengesellschaft, Germany
SOURCE:	PCT Int. Appl., 189 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9901160	A1	19990114	WO 1998-EP3142	19980527
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19728954	C1	19990422	DE 1997-19728954	19970630
AU 9882109	A	19990125	AU 1998-82109	19980527

PRIORITY APPLN. INFO.: DE 1997-19728954 A 19970630
WO 1998-EP3142 W 19980527

AB Conjugates PKm(LZ)n [P = polymer containing k amino groups; K = signal-generating chelating group containing metal ion; Z = mono- or oligosaccharide; L = linker; m, n = 1-149; k = 12-150; (m + n) ≤ k], optionally addnl. containing cations of inorg. and/or organic bases, amino acids, or amino acid amides, are valuable compds. for diagnosis and therapy, especially for NMR lymphog. These compds. are accumulated by lymph nodes and the lymphatic system sufficiently for good imaging, are well tolerated, have a low excretion time (generally >98% elimination within 14 days) and a high relaxivity, show no species-specific aberrations, and frequently allow morphol. differentiation of lymph node tissue. For diagnostic NMR imaging, the metal ion is paramagnetic; for therapeutic use of the conjugates, the metal ion is radioactive. Thus, DTPA monoanhydride mono-Et ester reacted with poly-L-lysine-HBr in aqueous solution at pH 9.5 to form a conjugate with a degree of substitution (d.s.) of 58.7% (47 DTPA units/mol.). This conjugate reacted with p-isothiocyanatophenyl-β-D-galactopyranose to produce a glycosyl conjugate with d.s. 41.1% (33 galactosyl residues/mol.). The glycosyl conjugate reacted with GdCl3 in aqueous buffer (pH 5.3) to produce the Gd chelate with no remaining free amino groups.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:642664 HCAPLUS
DOCUMENT NUMBER: 130:10828
TITLE: Renal Metabolism of 111In-DTPA-D-Phe1-Octreotide in Vivo
AUTHOR(S): Akizawa, Hiromichi; Arano, Yasushi; Uezono, Takashi; Ono, Masahiro; Fujioka, Yasushi; Uehara, Tomoya; Yokoyama, Akira; Akaji, Kenichi; Kiso, Yoshiaki; Koizumi, Mitsuru; Saji, Hideo
CORPORATE SOURCE: Department of Patho-Functional Bioanalysis Graduate School of Pharmaceutical Sciences, Kyoto University, Yoshida-Shimoadachi-cho Sakyo-ku Kyoto, 606-8501, Japan
SOURCE: Bioconjugate Chemistry (1998), 9(6), 662-670
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The persistent localization of radioactivity in the kidney after administration of 111In-DTPA-D-Phe1-octreotide impairs the diagnostic accuracy of this radiopharmaceutical. To better understand the mechanisms responsible for the renal radioactivity levels of 111In-DTPA-D-Phe1-octreotide, the renal metabolism of this compound was compared with 111In-DTPA-L-Phe1-octreotide, where the N-terminal D-phenylalanine was replaced with L-phenylalanine to facilitate metabolism DTPA-D-Phe1-octreotide and DTPA-L-Phe1-octreotide were synthesized by solid-phase methods. Both 111In-DTPA-conjugated octreotide analogs were prepared with radiochem. yields of over 96%, and both remained stable after a 3 h incubation in murine serum at 37°. When injected into mice, the two 111In-DTPA-conjugated octreotide analogs showed similar radioactivity elimination rates from the blood and accumulation in the kidney with about 60% injected radioactivity being excreted in the urine by 24 h postinjection. Over 85% of the radioactivity in the urine existed as intact peptides for both analogs. Despite the similar renal radioactivity

levels, significant differences were observed in the radiolabeled species remaining in the kidney between the two; while 111In-DTPA-L-Phe1-octreotide was rapidly metabolized to the final radiometabolite, 111In-DTPA-L-Phe, the metabolic rate of 111In-DTPA-D-Phe1-octreotide was so slow that various intermediate radiolabeled species were observed However, both 111In-DTPA-D-Phe and 111In-DTPA-L-Phe remained in the lysosomal compartment of the renal cells as the final radiometabolites for long periods. These findings indicated that although the metabolic stability of 111In-DTPA-D-Phe1-octreotide in the renal cells may be partially involved, the slow elimination rate of the radiometabolite derived from 111In-DTPA-D-Phe1-octreotide from the lysosomal compartment of renal cells would be predominantly attributable to the persistent renal radioactivity levels of 111In-DTPA-D-Phe1-octreotide.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:440582 HCAPLUS
DOCUMENT NUMBER: 129:245447
TITLE: Synthesis of metabolically stabilized peptides and their radiolabeling: new [111In]- and [*I]-neurotensin analogs
AUTHOR(S): Tourwe, D.; Mertens, J.; Ceusters, M.; Jeannin, L.; Iterbeke, K.; Terriere, D.; Chavatte, C.; Boumon, R.
CORPORATE SOURCE: Organic Chemistry Department, Vrije Universiteit Brussel, Brussels, B-1050, Belg.
SOURCE: Tumor Targeting (1998), 3(1), 41-45
CODEN: TUTAF9; ISSN: 1351-8488
PUBLISHER: Stockton Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Neurotensin (NT) is a neuropeptide which binds with high affinity to receptors in various tumors: small cell lung carcinoma, human colon and pancreas carcinoma and meningiomas. Radiolabeled analogs are therefore potentially useful for diagnosis and therapy. Because of rapid metabolism in vivo, metabolically stabilized analogs have to be prepared An approach is described based on the replacement of the scissile peptide bond by an isosteric ψ[CH2NH] function. For radioiodination using the Cu(I)-assisted nucleophilic exchange method, brominated benzoyl or phenylacetyl groups are attached to the N-terminus of NT(8-13). These retain high affinity for NT receptors and are radioiodinated with high radiochem. yield. For 111In labeling, DTPA was attached to the N-terminus of NT(8-13) using a monoreactive DTPA-tetra-tert-Bu ester. Labeling was performed in a kit formulation or NCA tracer was obtained after semi-prep HPLC. High affinity binding to NT receptors in guinea pig brain and in HT29 human adenocarcinoma cells was observed The stability in human plasma for [111In]DTPA-NT(8-13) was only 9.8 min, whereas that of the corresponding Lys8ψ[CH2NH]Arg9 analog exceeds 250 min.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:532575 HCAPLUS
DOCUMENT NUMBER: 127:135556
TITLE: Preparation of diaza-, triaza- and tetrazaalkane chelating agents for use as medicinal diagnostic and therapeutic agents
INVENTOR(S): Platzek, Johannes; Mareski, Peter; Niedballa, Ulrich;

	Raduechel, Bernd
PATENT ASSIGNEE(S):	Schering A.-G., Germany
SOURCE:	Ger. Offen., 11 pp.
	CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19601060	A1	19970710	DE 1996-19601060	19960104
DE 19601060	C2	20020425		
CA 2241825	A1	19970717	CA 1996-2241825	19961220
CA 2241825	C	20050927		
WO 9725305	A1	19970717	WO 1996-DE2476	19961220
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9718703	A	19970801	AU 1997-18703	19961220
EP 871608	A1	19981021	EP 1996-946110	19961220
EP 871608	B1	20000405		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000502715	T	20000307	JP 1997-524731	19961220
JP 3993235	B2	20071017		
AT 191456	T	20000415	AT 1996-946110	19961220
ES 2145517	T3	20000701	ES 1996-946110	19961220
PT 871608	T	20000731	PT 1996-946110	19961220
US 6080785	A	20000627	US 1998-101032	19980629
NO 9803103	A	19980703	NO 1998-3103	19980703
NO 322888	B1	20061218		
GR 3033822	T3	20001031	GR 2000-401522	20000629

PRIORITY APPLN. INFO.:	DE 1996-19601060	A	19960104
	WO 1996-DE2476	W	19961220

OTHER SOURCE(S): CASREACT 127:135556; MARPAT 127:135556

AB The title compds. A1NHCHR1CHR2(NA1CH2CH2)nNA12 and A1(A2)NCHR1CHR2(NA1CH2CH2)nNA12 [n = 0-2; A1 = CH2CO2CMe3; A2 = CH2CO2H; R1, R2 = H, or when n = 0 then R1R2 = (CH2)m; m = 3-6], useful as antidotes for heavy metal poisoning (no data), MRI diagnostics (no data), radiog. diagnostics (no data), and agents for radiotherapy (no data), are prepared by the alkylation of a properly blocked azaalkane with tert-Bu or lower-alkyl-leaving-group haloacetate esters, followed by lower-alkyl-leaving-group ester hydrolysis and removal of relevant blocking groups. Thus, 1,4,7-triazaheptane was protected with Et trifluoroacetate, the intermediate alkylated with tert-Bu bromoacetate, hydrolyzed with NH4OH, alkylated with benzyl bromoacetate, and the intermediate hydrogenated, producing di-tert-Bu 6,9-bis(tert-butoxycarbonylmethyl)-3-carboxymethyl-3,6,9-triazaundecanedicarboxylate.

L4 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1997:299305 HCAPLUS
DOCUMENT NUMBER:	126:317625
TITLE:	Conventional and High-Yield Synthesis of

DTPA-Conjugated Peptides: Application of a Monoreactive DTPA to DTPA-D-Phe1-octreotide Synthesis

AUTHOR(S): Arano, Yasushi; Akizawa, Hiromichi; Uezono, Takashi; Akaji, Kenichi; Ono, Masahiro; Funakoshi, Susumu; Koizumi, Mitsuru; Yokoyama, Akira; Kiso, Yoshiaki; Saji, Hideo

CORPORATE SOURCE: Dep. Radiopharm. Chem., Kyoto Univ., Kyoto, 606-01, Japan

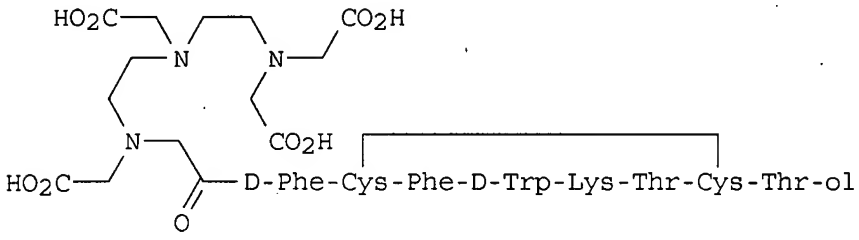
SOURCE: Bioconjugate Chemistry (1997), 8(3), 442-446
CODEN: BCCHES; ISSN: 1043-1802

PUBLISHER: American Chemical Society

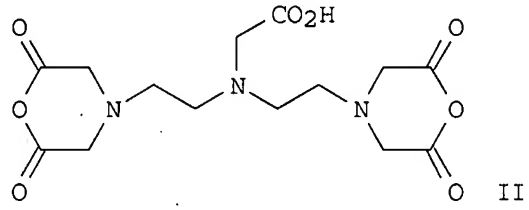
DOCUMENT TYPE: Journal

LANGUAGE: English

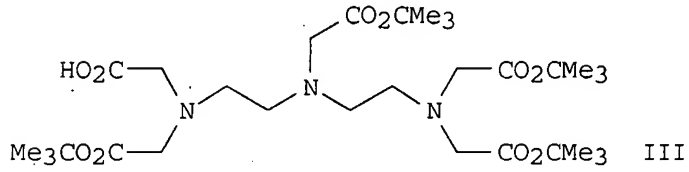
GI



I



II



III

AB Successful imaging of somatostatin receptor-pos. tumors with 111In-DTPA-D-Phe1-octreotide (111In-I) has stimulated development of peptide radiopharmaceuticals using DTPA as the chelating agent. However, use of cyclic DTPA dianhydride II resulted in low synthetic yields of DTPA-peptide by either solution or solid-phase syntheses. This paper reports a novel high-yield synthetic procedure for DTPA-D-Phe1-octreotide that is applicable to other peptides of interest using monoreactive DTPA derivative III. Monoreactive DTPA derivative III possesses one free terminal carboxylic acid along with four carboxylates protected with tert-Bu ester (mDTPA) was synthesized. N-9-Fluorenylmethoxycarbonyl-O-tert-butyl-L-threoninol (Fmoc-Thr(tBu)-ol), prepared from Fmoc-Thr(tBu)-OH, was loaded onto 2-chlorotrityl chloride resin. After construction of the peptide chains by Fmoc chemical, mDTPA was coupled to the α amine group of the peptide on the resin in the presence of 1,3-diisopropylcarbodiimide and

1-hydroxybenzotriazole. Treatment of the mDTPA-peptide-resin with trifluoroacetic acid-thioanisole removed the protecting groups and liberated [Cys(Acm)2,7]-octreotide-D-Phe1-DTPA from the resin. Iodine oxidation of the DTPA-peptide, followed by the reversed-phase HPLC purification, produced DTPA-D-Phe1-octreotide in overall 31.8% yield based on the starting Fmoc-Thr(tBu)-ol-resin. The final product gave a single peak on anal. HPLC, and amino acid anal. and mass spectrometry confirmed the integrity of the product. 111In radiolabeling of the product provided 111In-DTPA-D-Phe1-octreotide with >95% radiochem. yield, as confirmed by anal. reversed-phase HPLC, TLC, and CAE. These findings indicated that use of mDTPA during solid-phase peptide synthesis greatly increased the synthetic yield of DTPA-D-Phe1-octreotide, due to the absence of nonselective reactions that are unavoidable when cDTPA is used. These results also suggested that mDTPA would be a versatile reagent to introduce DTPA with high yield into peptides of interest.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:483602 HCAPLUS
DOCUMENT NUMBER: 125:162256
TITLE: Reassessment of Diethylenetriaminepentaacetic Dianhydride (DTPA) as a Chelating Agent for Indium-111 Labeling of Polypeptides Using a Newly Synthesized Monoreactive DTPA Derivative
AUTHOR(S): Arano, Yasushi; Uezono, Takashi; Akizawa, Hiromichi; Ono, Masahiro; Wakisaka, Kouji; Nakayama, Morio; Sakahara, Harumi; Konishi, Junji; Yokoyama, Akira
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kyoto University, Kyoto, 606-01, Japan
SOURCE: Journal of Medicinal Chemistry (1996), 39(18), 3451-3460
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Previous studies on indium-111 (111In) labeling of polypeptides and peptides using cyclic diethylenetriaminepentaacetic dianhydride (cDTPA) as a bifunctional chelating agent (BCA) have indicated that DTPA might be a useful BCA for 111In labeling of polypeptides at high specific activities when DTPA can be incorporated without inducing intra- or intermol. crosslinking. To investigate this hypothesis, a monoreactive DTPA derivative with a maleimide group as the peptide binding site (MDTPA) was designed and synthesized. A monoclonal antibody (OST7, IgG1) was used as a model polypeptide, and conjugation of MDTPA with OST7, 111In radiolabeling of MDTPA-OST7, and the stability of 111In-MDTPA-OST7 were investigated using cDTPA and benzyl-EDTA derivs. as refs. SDS-PAGE anal. demonstrated that while cDTPA induced intramol. crosslinking, no such undesirable side reactions were observed with MDTPA. MDTPA generated 111In-labeled OST7 with high radiochem. yields at higher specific activities than those produced using cDTPA and benzyl-EDTA derivs. as the BCAs. Incubation of each 111In-labeled OST7 in human serum indicated that MDTPA generated 111In-labeled OST7 of much higher and a little lower stability than those derived from cDTPA and benzyl-EDTA derivs., resp. These findings indicated that the low in vivo stability of cDTPA-conjugated antibody reported previously is not attributable to low stability of 111In-DTPA but to formation of intramol. crosslinking during cDTPA conjugation reactions.

The present study also indicated that MDTPA and its precursor, the tetra-tert-Bu derivative of DTPA, would be useful BCAs for 111In radiolabeling of polypeptides that have rapid blood clearance with high specific activities.

L4 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:267995 HCAPLUS
DOCUMENT NUMBER: 124:305630
TITLE: Dimeric DTPA derivatives and their metal complexes, pharmaceutical media containing these complexes, their use in der diagnostics and therapy and process for the preparation of the complexes and the media
INVENTOR(S): Krause, Werner; Maier, Franz-Karl; Bauer, Michael; Press, Wolf-Ruediger; Schuhmann-Giampieri, Gabriele; Platzek, Johannes; Schmitt-Willich, Heribert
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 25 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4428874	A1	19960222	DE 1994-4428874	19940808
US 5695737	A	19971209	US 1995-476117	19950607
CA 2197074	A1	19960222	CA 1995-2197074	19950808
WO 9605167	A1	19960222	WO 1995-EP3142	19950808
W: AU, BY, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RU, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9533433	A	19960307	AU 1995-33433	19950808
AU 695878	B2	19980827		
ZA 9506650	A	19960319	ZA 1995-6650	19950808
EP 775104	A1	19970528	EP 1995-929815	19950808
EP 775104	B1	19990506		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1156442	A	19970806	CN 1995-194571	19950808
JP 10503777	T	19980407	JP 1995-506999	19950808
HU 77532	A2	19980528	HU 1997-370	19950808
AT 179696	T	19990515	AT 1995-929815	19950808
ES 2134487	T3	19991001	ES 1995-929815	19950808
FI 9700535	A	19970207	FI 1997-535	19970207
NO 9700602	A	19970210	NO 1997-602	19970210
PRIORITY APPLN. INFO.:			DE 1994-4428874 A	19940808
			WO 1995-EP3142 W	19950808

AB Dimeric diethylenetriaminepentaacetic acid derivs. and their metal complexes (Z = 21-32, 37-39, 42-51, and 57-83) were prepared Contrast agents using these compds. were prepared for use in nuclear medicine.

=> file stng
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	61.80	235.46

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	-15.60	-15.60

FILE 'STNGUIDE' ENTERED AT 16:59:41 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 26, 2007 (20071026/UP).

=> d his

(FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007)

FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 5 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007
L4 20 S L3

FILE 'STNGUIDE' ENTERED AT 16:59:41 ON 29 OCT 2007

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.32	236.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-15.60

FILE 'CASREACT' ENTERED AT 17:13:04 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

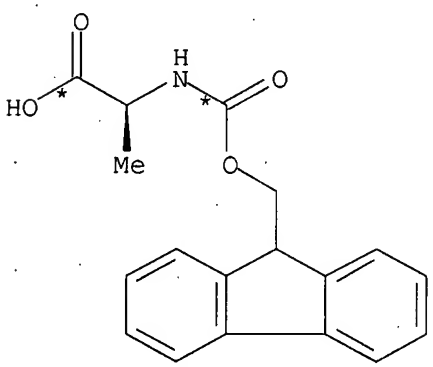
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
* *
* CASREACT now has more than 13.8 million reactions *
* *
****

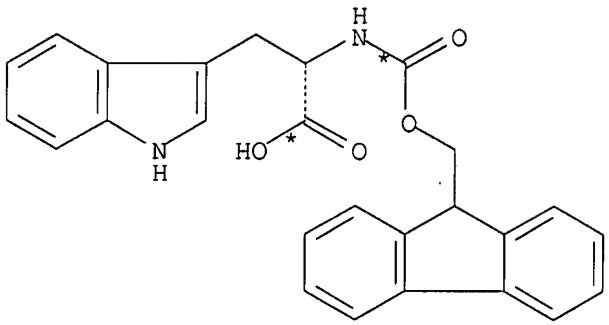
Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

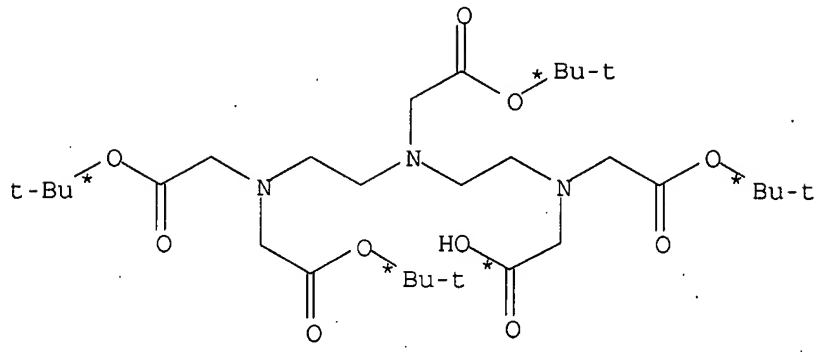
```
=> s l1
SAMPLE SEARCH INITIATED 17:13:10 FILE 'CASREACT'
SCREENING COMPLETE -       56 REACTIONS TO VERIFY FROM        7 DOCUMENTS

100.0% DONE      56 VERIFIED       0 HIT RXNS                          0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       672 TO     1568
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 sss full
FULL SEARCH INITIATED 17:13:31 FILE 'CASREACT'
SCREENING COMPLETE -     2593 REACTIONS TO VERIFY FROM      155 DOCUMENTS

100.0% DONE    2593 VERIFIED      17 HIT RXNS                          3 DOCS
SEARCH TIME: 00.00.01

L6            3 SEA SSS FUL L1 (    17 REACTIONS)

=> d l6 1-3 fhit

L6   ANSWER 1 OF 3  CASREACT  COPYRIGHT 2007 ACS on STN

RX(1) OF 13     A  +  B  +  C  ===>  D
```



A

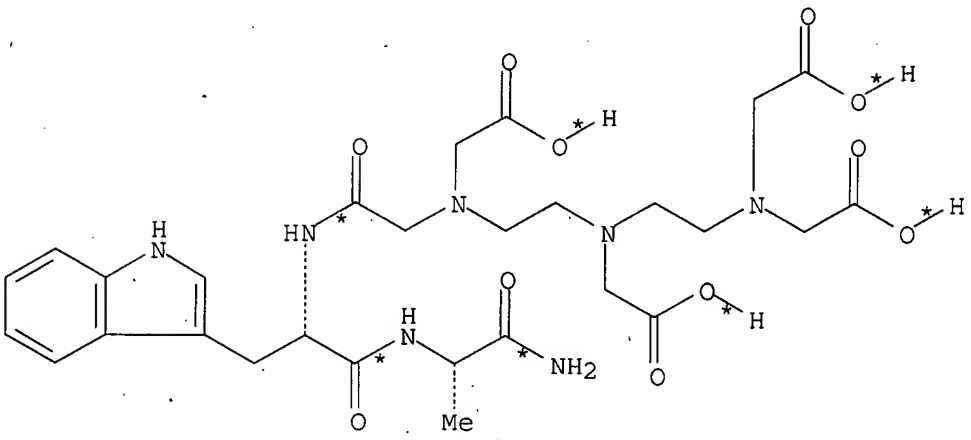


B



C

(1) →



D

RX(1) RCT A 35661-39-3

STAGE(1)
RGT E 125700-67-6 Benzotriazolium der, F 7087-68-5 EtN(Pr-i)2, G 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF
CON 1 - 3 hour, room temperature

STAGE(2)
RGT H 110-89-4 Piperidine
SOL 68-12-2 DMF
CON 15 - 30 minutes, room temperature

STAGE(3)
RCT B 35737-15-6
RGT E 125700-67-6 Benzotriazolium der, F 7087-68-5 EtN(Pr-i)2, G 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF
CON 1 - 3 hour, room temperature

STAGE(4)
RGT H 110-89-4 Piperidine
SOL 68-12-2 DMF
CON 15 - 30 minutes, room temperature

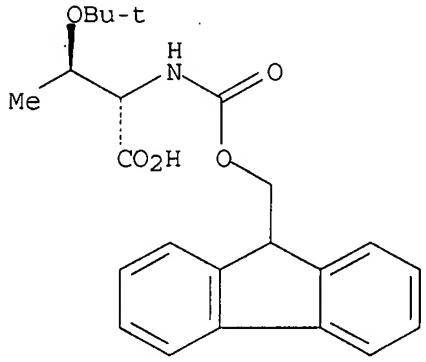
STAGE(5)
RCT C 180152-83-4
RGT E 125700-67-6 Benzotriazolium der, F 7087-68-5 EtN(Pr-i)2, G 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF
CON 1 - 3 hour, room temperature

STAGE(6)
RGT I 6485-79-6 Silane, tris(1-methylethyl)-, J 76-05-1 F3CCO2H
SOL 7732-18-5 Water
CON 3 hours, room temperature

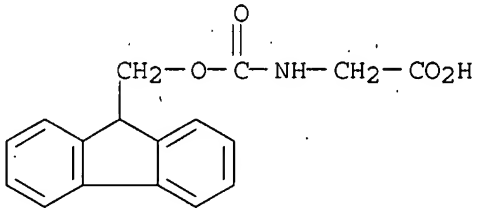
PRO D 899838-81-4
NTE solid-supported reaction, first stage attachment to Rink amide resin

L6 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

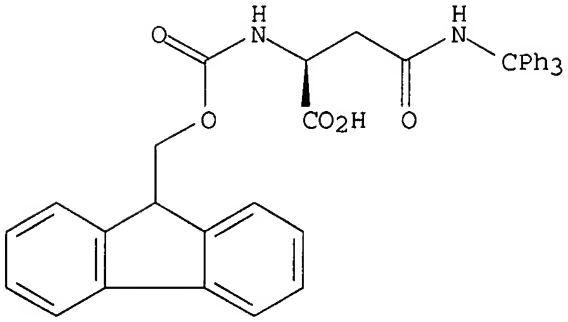
RX(1) OF 15 A + B + C + D + E + F ===> G...



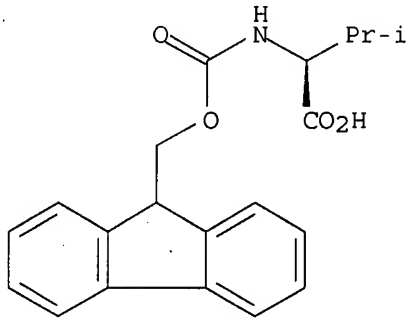
A



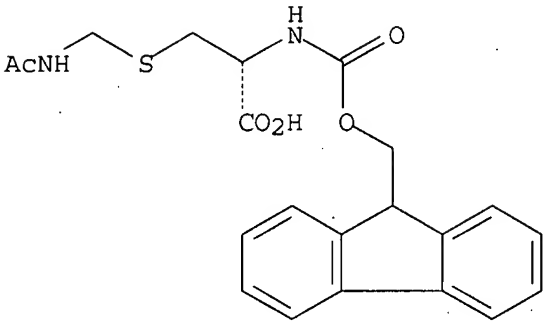
B



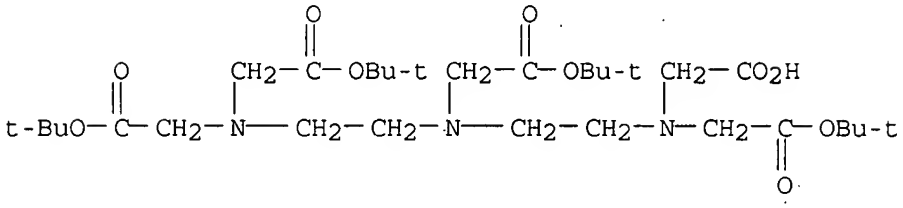
C



D


AcNH
S
H
N
O
CO2H
O

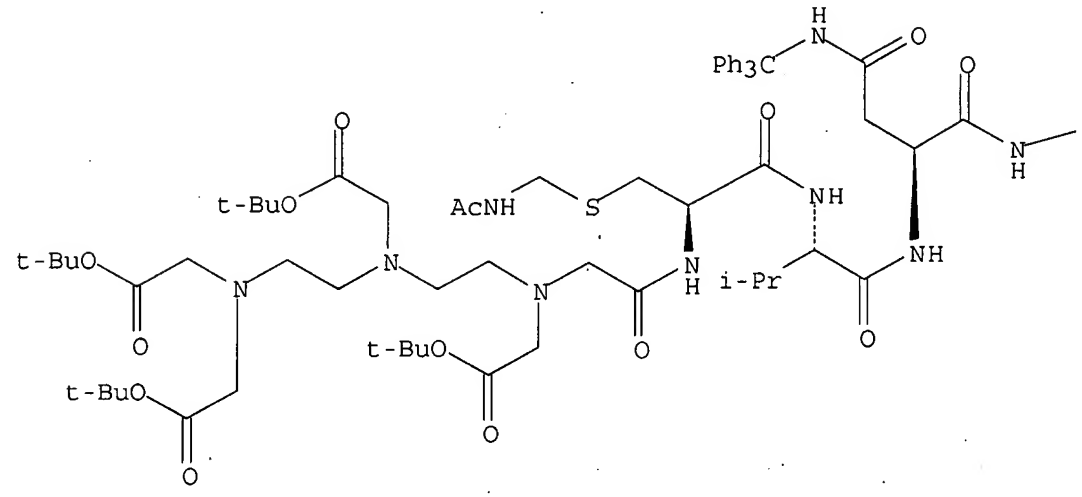
E

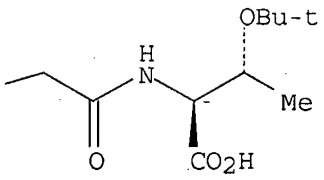

t-BuO
O
CH2
C
OBu-t
CH2
C
OBu-t
CH2
CO2H
N
CH2
CH2
N
CH2
CH2
N
CH2
C
OBu-t

F

(1)

PAGE 1-A


Ph3C
H
N
O
O
N
H
t-BuO
AcNH
S
NH
t-BuO
N
N
N
N
H
i-Pr
NH
t-BuO
t-BuO



G

RX(1) RCT A 71989-35-0

STAGE(1)

STAGE(2)
RCT B 29022-11-5

STAGE(3)
RCT C 132388-59-1

STAGE(4)
RCT D 68858-20-8

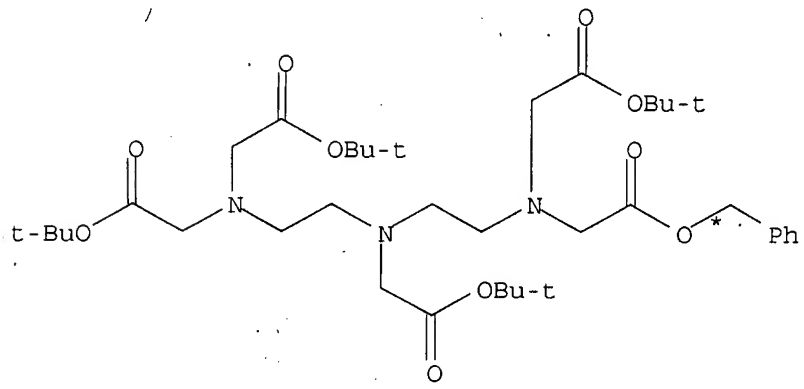
STAGE(5)
RCT E 86060-81-3

STAGE(6)
RCT F 180152-83-4

PRO G 796848-49-2
NTE no experimental detail, solid-supported reaction(first stage attachment to 2-chlorotrityl chloride resin)

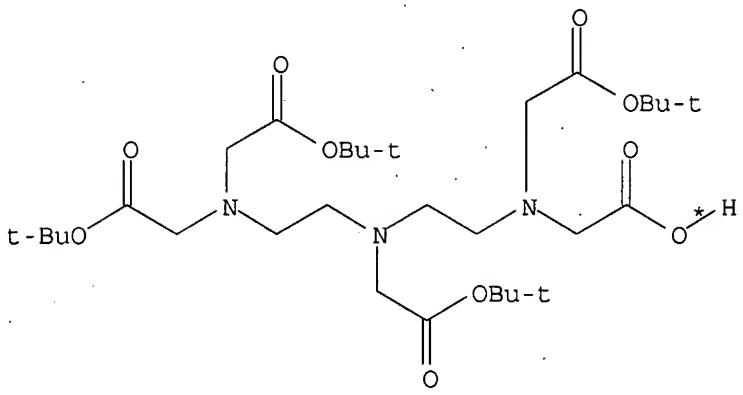
L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 2 A ===> B



A

(1)



B
YIELD 96%

RX(1) RCT A 180152-87-8
PRO B 180152-83-4
SOL 67-63-0 Me2CHOH
NTE 0-40.deg., H2

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	121.17	357.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-15.60

FILE 'STNGUIDE' ENTERED AT 17:14:52 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 26, 2007 (20071026/UP).

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.24	358.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-15.60

FILE 'STNGUIDE' ENTERED AT 17:17:00 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 26, 2007 (20071026/UP).

```
=> file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.06     358.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -15.60

FILE 'CASREACT' ENTERED AT 17:17:07 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 13.8 million reactions     *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d his

     (FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007)

     FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007
L1             STRUCTURE UPLOADED
L2           1 S L1
L3           5 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007
L4          20 S L3

     FILE 'STNGUIDE' ENTERED AT 16:59:41 ON 29 OCT 2007

     FILE 'CASREACT' ENTERED AT 17:13:04 ON 29 OCT 2007
L5           0 S L1
L6           3 S L1 SSS FULL

     FILE 'STNGUIDE' ENTERED AT 17:14:52 ON 29 OCT 2007

     FILE 'STNGUIDE' ENTERED AT 17:17:00 ON 29 OCT 2007
```

FILE 'CASREACT' ENTERED AT 17:17:07 ON 29 OCT 2007

=> d l6 1-3 ibib abs

L6 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 145:140459 CASREACT
TITLE: Phosphorylation State-Responsive Lanthanide Peptide Conjugates: A Luminescence Switch Based on Reversible Complex Reorganization
AUTHOR(S): Tremblay, Matthew S.; Zhu, Qing; Marti, Angel A.; Dyer, Joanne; Halim, Marlin; Jockusch, Steffen; Turro, Nicholas J.; Sames, Dalibor
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027; USA
SOURCE: Organic Letters (2006), 8(13), 2723-2726
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A luminogenic probe for peptide dephosphorylation has been developed. It consists of a serine-/tyrosine-containing peptide modified on the N-terminus with a tryptophan residue and a DTPA chelate capable of binding Tb3+. The authors propose a mechanistic model for the luminescence enhancement based on the interconversion of monomeric and dimeric lanthanide species, which is affected by the phosphorylation state of the serine or tyrosine residue. The optical switch reports effectively on phosphatase-catalyzed dephosphorylation in vitro.
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:421892 CASREACT
TITLE: De Novo Designed Peptidic Redox Potential Probe: Linking Sensitized Emission to Disulfide Bond Formation
AUTHOR(S): Lee, Kyung; Dzubeck, Valerie; Latshaw, Lauren; Schneider, Joel P.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716-2522, USA
SOURCE: Journal of the American Chemical Society (2004), 126(42), 13616-13617
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The design and utility of a peptidic probe capable of accurately measuring environmental redox potential via sensitized emission has been prepared This probe is characterized by long-lived luminescence (millisecond), nanomolar detection limits, and a probe reduction potential of -0.243 V.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 127:135556 CASREACT
TITLE: Preparation of diaza-, triaza- and tetrazaalkane

chelating agents for use as medicinal diagnostic and therapeutic agents

INVENTOR(S): Platzek, Johannes; Mareski, Peter; Niedballa, Ulrich; Raduechel, Bernd

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19601060	A1	19970710	DE 1996-19601060	19960104
DE 19601060	C2	20020425		
CA 2241825	A1	19970717	CA 1996-2241825	19961220
CA 2241825	C	20050927		
WO 9725305	A1	19970717	WO 1996-DE2476	19961220
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9718703	A	19970801	AU 1997-18703	19961220
EP 871608	A1	19981021	EP 1996-946110	19961220
EP 871608	B1	20000405		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000502715	T	20000307	JP 1997-524731	19961220
JP 3993235	B2	20071017		
AT 191456	T	20000415	AT 1996-946110	19961220
ES 2145517	T3	20000701	ES 1996-946110	19961220
PT 871608	T	20000731	PT 1996-946110	19961220
US 6080785	A	20000627	US 1998-101032	19980629
NO 9803103	A	19980703	NO 1998-3103	19980703
NO 322888	B1	20061218		
GR 3033822	T3	20001031	GR 2000-401522	20000629
PRIORITY APPLN. INFO.:			DE 1996-19601060	19960104
			WO 1996-DE2476	19961220

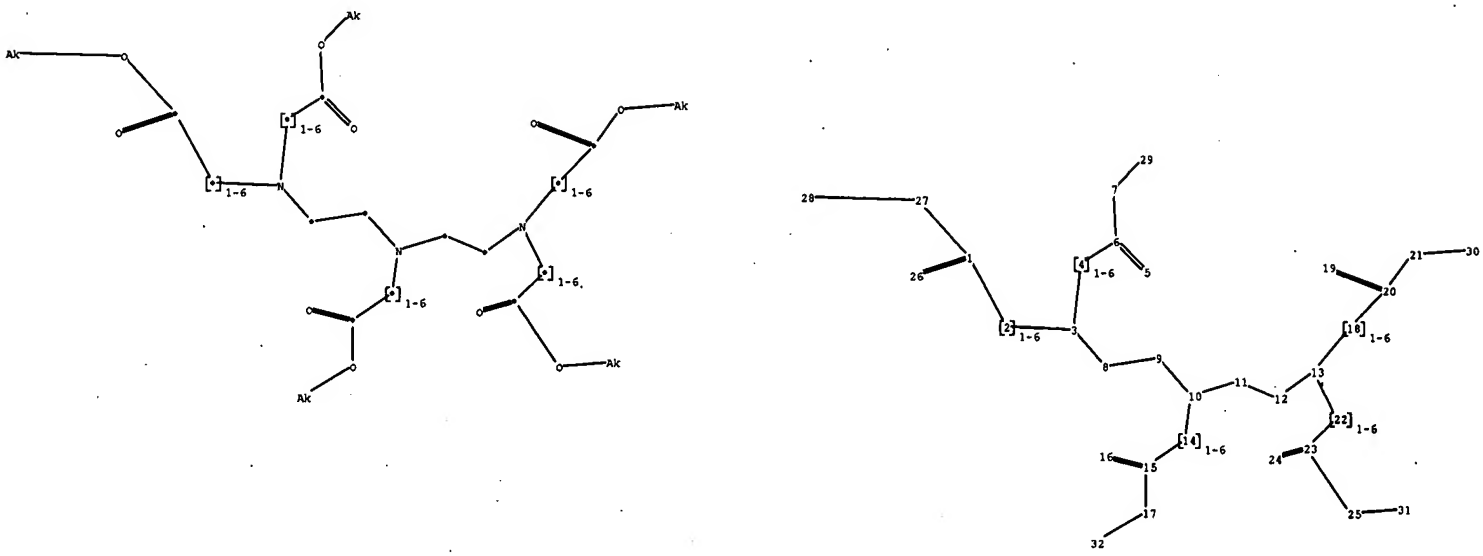
OTHER SOURCE(S): MARPAT 127:135556

AB The title compds. A1NHCHR1CHR2(NA1CH2CH2)nNA12 and A1(A2)NCHR1CHR2(NA1CH2CH2)nNA12 [n = 0-2; A1 = CH2CO2CMe3; A2 = CH2CO2H; R1, R2 = H, or when n = 0 then R1R2 = (CH2)m; m = 3-6], useful as antidotes for heavy metal poisoning (no data), MRI diagnostics (no data), radiog. diagnostics (no data), and agents for radiotherapy (no data), are prepared by the alkylation of a properly blocked azaalkane with tert-Bu or lower-alkyl-leaving-group haloacetate esters, followed by lower-alkyl-leaving-group ester hydrolysis and removal of relevant blocking groups. Thus, 1,4,7-triazaheptane was protected with Et trifluoroacetate, the intermediate alkylated with tert-Bu bromoacetate, hydrolyzed with NH4OH, alkylated with benzyl bromoacetate, and the intermediate hydrogenated, producing di-tert-Bu 6,9-bis(tert-butoxycarbonylmethyl)-3-carboxymethyl-3,6,9-triazaundecanedicarboxylate.

```
=> file stng
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     8.49     366.74

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -2.19     -17.79

FILE 'STNGUIDE' ENTERED AT 17:17:58 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 26, 2007 (20071026/UP).

=> file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.42     367.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -17.79

FILE 'CASREACT' ENTERED AT 17:22:03 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*     CASREACT now has more than 13.8 million reactions    *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> s l1/pro
QUALIFICATION NOT VALID FOR L1
Field code qualifications can only be applied to text
terms.

=> d his
```

```
     (FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007)

     FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007
L1                STRUCTURE UPLOADED
L2              1 S L1
L3              5 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007
L4             20 S L3

     FILE 'STNGUIDE' ENTERED AT 16:59:41 ON 29 OCT 2007

     FILE 'CASREACT' ENTERED AT 17:13:04 ON 29 OCT 2007
L5              0 S L1
L6              3 S L1 SSS FULL

     FILE 'STNGUIDE' ENTERED AT 17:14:52 ON 29 OCT 2007

     FILE 'STNGUIDE' ENTERED AT 17:17:00 ON 29 OCT 2007

     FILE 'CASREACT' ENTERED AT 17:17:07 ON 29 OCT 2007

     FILE 'STNGUIDE' ENTERED AT 17:17:58 ON 29 OCT 2007

     FILE 'CASREACT' ENTERED AT 17:22:03 ON 29 OCT 2007
```

C:\Program Files\Stnexp\Queries\2007 cases\10766470\generic molecule diethylenetriamine deriv.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32

chain bonds :

1-2 1-26 1-27 2-3 3-4 3-8 4-6 5-6 6-7 7-29 8-9 9-10 10-11 10-14 11-12 12-13 13-18 13-22 14-15 15-16 15-17 17-32 18-20 19-20 20-21 21-30 22-23 23-24 23-25 25-31 27-28

exact/norm bonds :

1-26 1-27 2-3 3-4 3-8 5-6 6-7 7-29 9-10 10-11 10-14 12-13 13-18 13-22 15-16 15-17 17-32 19-20 20-21 21-30 23-24 23-25 25-31 27-28

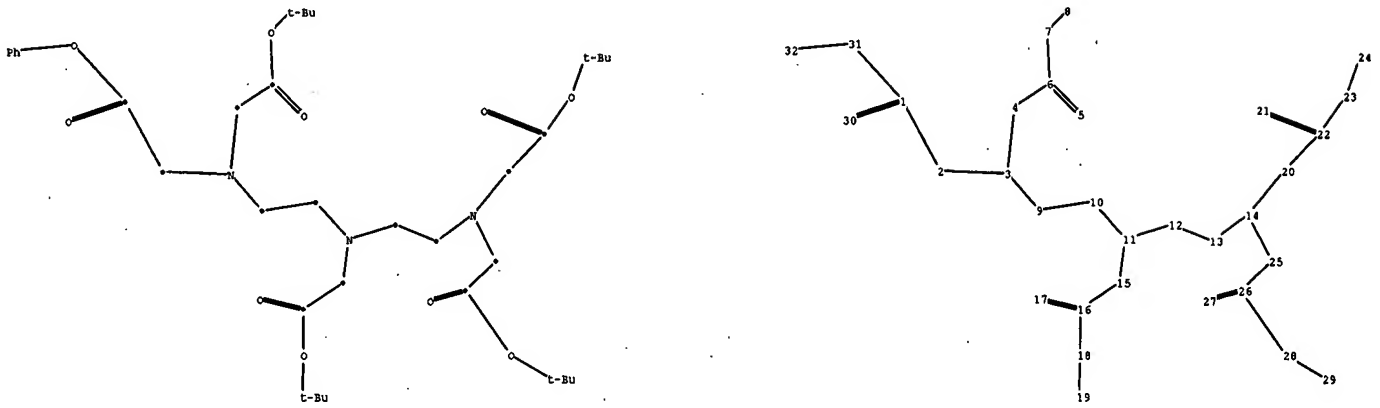
exact bonds :

1-2 4-6 8-9 11-12 14-15 18-20 22-23

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS

C:\Program Files\Stnexp\Queries\2007 cases\10766470\molecule VI cl128.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32

chain bonds :
1-2 1-30 1-31 2-3 3-4 3-9 4-6 5-6 6-7 7-8 9-10 10-11 11-12 11-15 12-13 13-14 14-20 14-25 15-16 16-17 16-18 18-19 20-22 21-22 22-23 23-24 25-26 26-27 26-28 28-29 31-32

exact/norm bonds :
1-30 1-31 2-3 3-4 3-9 5-6 6-7 10-11 11-12 11-15 13-14 14-20 14-25 16-17 16-18 21-22 22-23 26-27 26-28

exact bonds :
1-2 4-6 7-8 9-10 12-13 15-16 18-19 20-22 23-24 25-26 28-29 31-32

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS